

# Density Functional Theory of Bosons in a Trap

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A time-dependent Kohn-Sham (KS) like theory is presented for  $N$  bosons in three and lower-dimensional traps. We derive coupled equations, which allow one to calculate the energies of elementary excitations. A rigorous proof is given to show that the KS like equation correctly describes properties of the one-dimensional condensate of impenetrable bosons in a general time-dependent harmonic trap in the large  $N$  limit.

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The newly created Bose-Einstein condensates (BEC) of weakly interacting alkali-metal atoms [1] stimulated a large number of theoretical investigations (see recent reviews [2]). Most of these works are based on the assumption that the properties of BEC are well described by the Gross-Pitaevskii (GP) mean-field theory [3]. The validity of the GP equation is nearly universally accepted.

The experimental realization of quasi-one dimensional (1D) and quasi-two dimensional (2D) trapped gases [4-6] stimulated many theoretical interests. The theoretical aspects of the BEC in quasi-1D and quasi-2D traps have been reported in many papers [7-17]. For the case of dimensions  $d < 3$ , it is known that the quantum-mechanical two-body  $t$ -matrix vanishes [18] at low energies. Therefore the replacement of the two-body interaction by the  $t$ -matrix, as done in deriving the GP mean-field theory, is not correct in general for  $d < 3$  [12,19].

The density functional theory (DFT), originally developed for interacting systems of fermions [20], provides a rigorous alternative approach to the interacting inhomogeneous Bose gases. The main goal of this letter is to develop a Kohn-Sham (KS) like time-dependent theory for bosons.

We consider a system of  $N$  interacting bosons in a trap potential  $V_{ext}$ . Assuming that our system is in a local thermal equilibrium at each position  $\vec{r}$  with the local energy per particle  $\epsilon(n)$  ( $\epsilon$  is the ground state energy per particle of the homogeneous system and  $n$  is the density), we can write a zero temperature classical hydrodynamics equation as [8]

$$\frac{\partial n}{\partial t} + \nabla(n\vec{v}) = 0, \quad (1)$$

$$\frac{\partial \vec{v}}{\partial t} + \frac{1}{m}\nabla(V_{ext} + \frac{\partial(n\epsilon(n))}{\partial n} + \frac{1}{2}m\vec{v}^2) = 0, \quad (2)$$

where  $\vec{v}$  is the velocity field.

Adding the kinetic energy pressure term, we have

$$\frac{\partial \vec{v}}{\partial t} + \frac{1}{m}\nabla(V_{ext} + \frac{\partial(n\epsilon(n))}{\partial n} + \frac{1}{2}m\vec{v}^2 - \frac{\hbar^2}{2m}\frac{1}{\sqrt{n}}\nabla^2\sqrt{n}) = 0. \quad (3)$$

We define the density of the system as

$$n(\vec{r}, t) = |\Psi(\vec{r}, t)|^2, \quad (4)$$

and the velocity field  $\vec{v}$  as

$$\vec{v}(\vec{r}, t) = \frac{\hbar}{2imn(\vec{r}, t)}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*). \quad (5)$$

From Eqs.(1) and (5), we obtain the following KS like time-dependent equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V_{ext} \Psi + \frac{\partial(n\epsilon(n))}{\partial n} \Psi. \quad (6)$$

If the trap potential,  $V_{ext}$ , is independent of time, one can write the ground-state wave function as  $\Psi(\vec{r}, t) = \Phi(\vec{r}) \exp(-i\mu t/\hbar)$ , where  $\mu$  is the chemical potential, and  $\Phi$  is normalized to the total number of particles,  $\int d\vec{r} |\Phi|^2 = N$ . Then Eq.(6) becomes [21]

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{ext} + \frac{\partial(n\epsilon(n))}{\partial n}\right) \Phi = \mu \Phi, \quad (7)$$

where the solution of the equation (7) minimizes the KS energy functional in the local density approximation (LDA)

$$E = N \langle \Phi | -\frac{\hbar^2}{2m} \nabla^2 + V_{ext} + \epsilon(n) | \Phi \rangle, \quad (8)$$

and the chemical potential  $\mu$  is given by  $\mu = \partial E / \partial N$ . Eq.(7) has the form of the KS equation.

The ground-state energy per particle of the homogeneous system  $\epsilon(n)$  for dilute 3D [22] and dilute 2D [23] Bose gases are

$$\epsilon(n) = \frac{2\pi\hbar^2}{m} a_{3D} n \left[ 1 + \frac{128}{15\sqrt{\pi}} (na_{3D}^3)^{1/2} + 8\left(\frac{4\pi}{3} - \sqrt{3}\right) na_{3D}^3 \ln(na_{3D}^3) + \dots \right], \quad (9)$$

and

$$\epsilon(n) = \frac{2\pi\hbar^2 n}{m} |\ln(na_{2D}^2)|^{-1} (1 + O(|\ln(na_{2D}^2)|^{-1/5})), \quad (10)$$

where  $a_{3D}$  and  $a_{2D}$  are 3D and 2D scattering lengths respectively.

For 1D Bose gas interacting via a repulsive  $\delta$ -function potential,  $\tilde{g}\delta(x)$ ,  $\epsilon(n)$  is given by [24]

$$\epsilon(n) = \frac{\hbar^2}{2m} n^2 e(\gamma), \quad (11)$$

where  $\gamma = m\tilde{g}/(\hbar^2 n)$  and

$$e(\gamma) = \frac{\gamma^3}{\lambda^3} \int_{-1}^{+1} g(x) x^2 dx, \quad (12)$$

$$g(y) = \frac{1}{2\pi} \left( 1 + 2\lambda \int_{-1}^{+1} \frac{g(x) dx}{\lambda^2 + (x-y)^2} \right),$$

$$\lambda = \gamma \int_{-1}^{+1} g(x) dx.$$

For small values of  $\gamma$ , the following expression for  $\epsilon(n)$ ,

$$\epsilon(n) = \frac{\tilde{g}}{2}(n - \frac{4}{3\pi}\sqrt{\frac{m\tilde{g}n}{\hbar^2}}) + \dots \quad (13)$$

is adequate up to approximately  $\gamma = 2$  [24].

For a large coupling strength  $\tilde{g}$  [24]

$$\epsilon(n) = \frac{\hbar^2 \pi^2 n^2}{6m} (1 + \frac{2\hbar^2 n}{m\tilde{g}})^{-2}. \quad (14)$$

Eq.(14) is accurate to 1% for  $\gamma \geq 10$  [24].

In the limit of large  $N$ , by neglecting the kinetic energy term in the KS equation (7), we obtain an equation corresponding to the Thomas-Fermi (TF) approximation

$$V_{ext} + \frac{\partial(n\epsilon(n))}{\partial n} = \mu \quad (15)$$

in the region where  $n(\vec{r})$  is positive and  $n(\vec{r}) = 0$  outside this region.

Now we turn our attention to elementary excitations, corresponding to small oscillations of  $\Psi(\vec{r}, t)$  around the ground state. Elementary excitations can be obtained by standard linear response analysis [25,26] of the equation (6), as resonances in the linear response. We add a weak sinusoidal perturbation to the time-dependent equation (6)

$$i\hbar \frac{\partial \Psi}{\partial t} = (-\frac{\hbar^2}{2m} \nabla^2 + V_{ext} + \frac{\partial(n\epsilon(n))}{\partial n} + f_+ e^{-i\omega t} + f_- e^{i\omega t}) \Psi, \quad (16)$$

and assume that solution of Eq.(16) has the following form

$$\Psi(\vec{r}, t) = e^{-i\mu t/\hbar} [\Phi(\vec{r}) + u(\vec{r})e^{-i\omega t} + v^*(\vec{r})e^{i\omega t}], \quad (17)$$

where  $\Phi(\vec{r})$  is the ground-state solution of Eq.(7).

Linearization in small amplitudes  $u$  and  $v$  yields inhomogeneous equations

$$\begin{aligned} (L - \hbar\omega)u + \frac{\partial^2(n\epsilon(n))}{\partial n^2} \Phi^2 v &= -f_+ \Phi, \\ (L + \hbar\omega)v + \frac{\partial^2(n\epsilon(n))}{\partial n^2} \Phi^{*2} u &= -f_- \Phi, \end{aligned} \quad (18)$$

where  $n = |\Phi(\vec{r})|^2$  and

$$L = -\frac{\hbar^2}{2m} \nabla^2 + V_{ext} - \mu + \frac{\partial(n\epsilon(n))}{\partial n} + \frac{\partial^2(n\epsilon(n))}{\partial n^2} n. \quad (19)$$

Setting  $f_{\pm}$  to zero in Eq.(18), we obtain coupled equations

$$\begin{aligned} Lu + \frac{\partial^2(n\epsilon(n))}{\partial n^2} \Phi^2 v &= \hbar\omega u, \\ Lv + \frac{\partial^2(n\epsilon(n))}{\partial n^2} \Phi^{*2} u &= -\hbar\omega v, \end{aligned} \quad (20)$$

which can be used to calculate the energies  $\mathcal{E} = \hbar\omega$  of the elementary excitations.

Now we describe the application of the time-dependent equation (6) to the case of non-linear dynamics. We turn to the limit of very strong coupling between the interacting bosons in  $1D$ , the so-called Tonks-Girardeau gas [27]. In this impenetrable bosons case, the energy density  $\epsilon(n)$ , Eq.(13), reduces to  $\epsilon(n) = \hbar^2 \pi^2 n^2 / 6m$ , and Eq.(6) reads [12]

$$i\hbar \frac{\partial \Psi}{\partial t} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_{ext} + \frac{\hbar^2 \pi^2}{2m} |\Psi|^4 \right) \Psi, \quad (21)$$

with  $\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = N$ .

For a general time-dependent harmonic trap  $V_{ext} = m\omega^2(t)x^2/2$ , with the initial condition  $\Psi(x, 0) = \Phi(x)$ , where  $\Phi(x)$  is the ground-state solution of the time-independent equation

$$\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2(0)x^2}{2} + \frac{\hbar^2 \pi^2}{2m} |\Phi|^4 \right) \Phi = \mu \Phi, \quad (22)$$

we show that Eq.(21) reduces to the ordinary differential equations which can provide the exact solution of Eq.(21).

Indeed, if we assume that the solution,  $\Psi(x, t)$ , can be expressed as

$$\Psi(x, t) = \frac{\Phi(x/\lambda(t))}{\sqrt{\lambda(t)}} e^{-i\beta(t) + im \frac{x^2}{2\hbar} \frac{\dot{\lambda}}{\lambda}}, \quad (23)$$

we obtain the following equations for  $\lambda$  and  $\beta$  after inserting Eq.(23) into Eq.(21):

$$\ddot{\lambda} + \omega^2(t)\lambda = \frac{\omega^2(0)}{\lambda^3}, \quad \lambda(0) = 1, \quad \dot{\lambda}(0) = 0, \quad (24)$$

$$\dot{\beta} = \frac{\mu}{\hbar\lambda^2}, \quad \beta(0) = 0. \quad (25)$$

Thus, the ordinary differential equations Eqs.(22), (24), and (25) give the exact solution of Eq.(21), and the evolution of the density can be written exactly as

$$n(x, t) = (1/\lambda(t))n(x/\lambda(t), 0). \quad (26)$$

For the case of free expansion, the confining potential is switched off at  $t = 0$  and the atoms fly away. In this case, Eqs.(24) and (25) can be integrated analytically leading to the following solutions for  $\lambda$  and  $\beta$ :

$$\lambda(t) = \sqrt{1 + \omega^2(0)t^2}, \quad \beta(t) = \frac{\mu}{\hbar\omega(0)} \arctan(\omega(0)t). \quad (27)$$

We note that self-similar solutions [28] of Eq.(21) were briefly discussed in Ref.[29].

In the large  $N$  limit, where the kinetic energy term in Eq.(22) is dropped altogether (the so-called Thomas-Fermi limit), the corresponding density is

$$n_{TF}(x, t) = \frac{1}{\pi\tilde{\lambda}(t)} [(2N - \frac{x^2}{\tilde{\lambda}^2(t)})]^{1/2} \theta(2N - \frac{x^2}{\tilde{\lambda}^2(t)}), \quad (28)$$

and for the Fourier transform  $n(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} n(x, t) e^{ikx} dx$  we have

$$n_{TF}(k, t) = \frac{N}{\sqrt{2\pi}} \frac{2J_1(\sqrt{2N}\tilde{\lambda}(t)k)}{\sqrt{2N}\tilde{\lambda}(t)k}, \quad (29)$$

where  $\tilde{\lambda}(t) = [\hbar/(m\omega(0))]^{1/2}\lambda(t)$  and  $J_1$  is the Bessel function of the first order.

The exact many-body wave function,  $\Psi_B(x_1, x_2, \dots, x_N, t)$ , of a system of  $N$  impenetrable bosons in a time dependent 1D harmonic trap, can be found from the Fermi-Bose mapping [15]

$$|\Psi_B(x_1, x_2, \dots, x_N, t)| = |\Psi_F(x_1, x_2, \dots, x_N, t)|, \quad (30)$$

where  $\Psi_F$  is the fermionic solution of the time-dependent many-body Schrödinger equation

$$i\hbar \frac{\partial \Psi_F}{\partial t} = \sum_{i=1}^N \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{m\omega^2(t)x_i^2}{2} \right) \Psi_F. \quad (31)$$

with initial condition  $\Psi_F(x_1, x_2, \dots, x_N, 0) = \Phi_F(x_1, x_2, \dots, x_N)$ , where  $\Phi_F(x_1, x_2, \dots, x_N)$  is the fermionic ground-state solution of the time-independent Schrödinger equation

$$\sum_{i=1}^N \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{m\omega^2(0)x_i^2}{2} \right) \Phi_F = E\Phi_F.$$

Therefore, for the exact density  $n_B(x, t) = \int_{-\infty}^{+\infty} dx_2 \dots \int_{-\infty}^{+\infty} dx_N |\Psi_B(x, x_2, \dots, x_N, t)|^2$ , we have

$$n_B(x, t) = \frac{1}{\tilde{\lambda}(t)} \sum_{i=0}^{N-1} \left| \phi_i\left(\frac{x}{\tilde{\lambda}(t)}\right) \right|^2, \quad (32)$$

where  $\phi_i(x) = c_i \exp(-x^2/2) H_i(x)$ ,  $c_i = \pi^{-1/4} (2^i i!)^{-1/2}$ , and  $H_i(x)$  are Hermite polynomials. Note that the evolution of  $n_B(x, t)$  can be written as Eq.(26), corresponding to a time-dependent dilatation of length scale.

From the knowledge of  $n_B(x, t)$  and  $n_{TF}(x, t)$  one can evaluate the radii  $r(t) = (\int_{-\infty}^{+\infty} n_B(x, t)x^2 dx)^{1/2}$  and  $r_{TF}(t) = (\int_{-\infty}^{+\infty} n_{TF}(x, t)x^2 dx)^{1/2}$  and ratio  $r(t)/r_{TF}(t)$ . This quantity is equal to 1 at any  $t$  for any  $N$ . This circumstance explains why for a harmonic trap the ground-state density profile from Eq.(21) agrees well with the many-body results for systems with a rather small number of atoms  $N \approx 10$  [12]. As for a general trap potential we expect such agreement for much larger  $N$ .

Using the following relation [30]

$$\sum_{m=0}^n (2^m m!)^{-1} [H_m(x)]^2 = (2^{n+1} n!)^{-1} \{[H_{n+1}(x)]^2 - H_n(x)H_{n+2}(x)\}, \quad (33)$$

we obtain an analytical formula for exact density  $n_B(x, t)$

$$n_B(x, t) = \frac{1}{2\tilde{\lambda}(t)} c_{N-1}^2 e^{-x^2/\tilde{\lambda}^2(t)} \{[H_N(x/\tilde{\lambda}(t))]^2 - H_{N-1}(x/\tilde{\lambda}(t))H_{N+1}(x/\tilde{\lambda}(t))\}. \quad (34)$$

Then the Fourier transform is given by

$$n_B(k, t) = \frac{1}{\sqrt{2\pi}} e^{-\tilde{\lambda}^2(t)k^2/4} [NL_N^{(0)}(\frac{\tilde{\lambda}^2(t)k^2}{2}) + \frac{\tilde{\lambda}^2(t)k^2}{2} L_{N-1}^{(2)}(\frac{\tilde{\lambda}^2(t)k^2}{2})], \quad (35)$$

where  $L_n^{(\alpha)}$  are Laguerre polynomials. Using the asymptotic formula of Hilb's type for the Laguerre polynomial [30], we have the asymptotic behavior of  $n_B(k, t)$  as  $N \rightarrow \infty$

$$n_B(k, t) = \frac{N}{\sqrt{2\pi}} \frac{2J_1(\sqrt{2N}\tilde{\lambda}(t)k)}{\sqrt{2N}\tilde{\lambda}(t)k} + O(N^{1/4}), \quad (36)$$

which is valid uniformly in any bounded region of  $k\tilde{\lambda}(t)$ . Eq.(36) for the case of  $t = 0$  is a rigorous justification of the Thomas-Fermi approximation [13,31] to a system of non-interacting 1D spinless fermions in harmonic trapping potentials.

Comparison of Eq.(36) with Eq.(29) shows that in the large  $N$  limit the KS like time-dependent theory for 1D impenetrable bosons in a time-dependent harmonic trap, Eq.(29), gives the same result as the exact many-body treatment, Eq.(36). Hence, we have rigorously proved that Eq.(29) correctly describes properties of 1D Bose gas in a time-dependent harmonic trap in the limit of large  $N$ .

In conclusion, we have developed a time-dependent KS like theory for bosons in three and lower-dimensional traps and have obtained coupled equations which can be used to calculate the energies of elementary excitations. For one-dimensional condensate of impenetrable

bosons in a general time-dependent harmonic trap, it is shown that the corresponding equation reduces to the ordinary differential equations and gives the same results as the exact many-body treatment in the large  $N$  limit.

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